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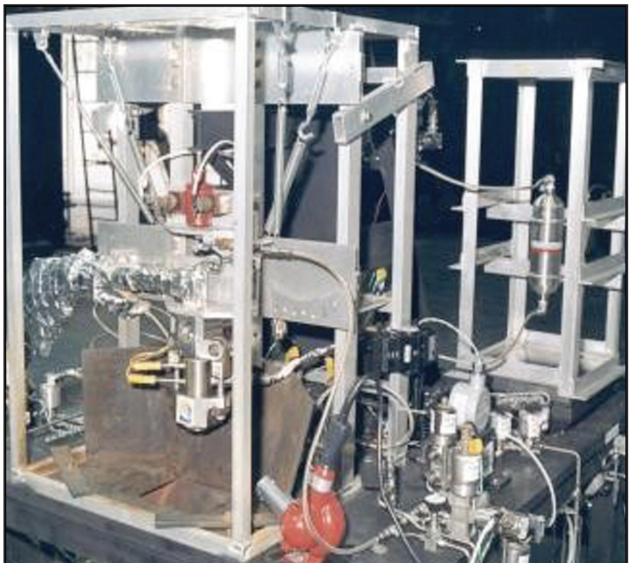
Science and Technology for Tomorrow's Air and Space Force

Success Story

TOXICITY OF HIGH-ENERGY CHEMICALS



A collaborative study between the Human Effectiveness Directorate (HE) and the Materials and Manufacturing Directorate (ML), using cellular and computational studies supported by the Air Force Office of Scientific Research, enabled a risk assessment for new high-energy chemicals synthesized in the Propulsion Directorate (PR). Experimental testing by HE, combined with the theoretical work by ML, can reduce the time and cost of toxicity evaluations for potential new propellants.

The combined experimental and computational studies outlined a paradigm for a first-level toxicity screening of new chemicals and propellants of interest to the Air Force. A potential replacement for the highly toxic hydrazine monopropellant is possible as a result of the synthesis and assessment of this new class of high-energy chemicals.

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Accomplishment

Drs. Tom Hawkins and Jerry Boatz, both of PR, designed a new class of hydrazine salts and, together with Mr. Adam Brand of PR, synthesized and characterized 13 high-energy chemicals. Drs. Saber Hussain and John Frazier, both of HE, in collaboration with Drs. Steve Trohalaki and Ruth Pachter, both of ML, carried out the test battery of end points and developed the Quantitative Structure Activity Relationship (QSAR) models. QSARs enable the screening of the new class of high-energy chemicals for potential toxicity and rank them with respect to hydrazine, a highly toxic monopropellant.

Background

Researchers must often use animal tests to assess the toxicity of a chemical. However, due to the cost and time involved in toxicological assessments, early toxicity screening of new chemicals is important in predicting the adverse effects of chemical compounds. At the earliest stage of toxicity screening, biochemical toxicity end points, combined with computational studies, aid in decisions regarding development of novel chemicals, such as new propellants, by the Air Force.

HE scientists measured the following end points in primary cultures of isolated rat liver cells: mitochondrial function, lactate dehydrogenase leakage, generation of reactive oxygen species, and reduced glutathione content. The experimental results demonstrate that hydrazine-based compounds are more toxic than amine and triazole-containing compounds. Researchers could rank hydrazine-based compounds in order of decreasing toxicity with respect to hydrazine. Using theoretical calculated molecular descriptors, ML researchers derived QSARs for the biochemical toxicity end points. Application of the derived QSARs will assist in predicting toxicity for newly proposed propellants.

Human Effectiveness
Emerging Technologies

Additional information

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